Abstract No. ozca738

Microstructure Evolution in Ti-Ta Thin Films on Si(001) and Poly-Si

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Beamline(s): X20C

Introduction: Titanium disilicide has been used widely in Si ultra-large-scale integration (ULSI) technology because of its low resistivity and relatively high thermal stability. $TiSi_2$ exists in two polymorphs, with crystallographic designations C49 and C54. The C54 phase, which has a face-centered orthorhombic unit cell has a significantly lower resistivity (15-20 $\mu\Omega$-cm) than does the C49 structure (60-75 $\mu\Omega$-cm), which has a base-centered orthorhombic unit cell. Although the technologically desired C54 phase is the equilibrium phase of the disilicide, under most conditions the C49 phase is kinetically favored. The transformation to the C54 phase can be difficult, particularly in submicron features. Interposing a thin layer of a refractory metal has been found to be effective in reducing the C54 transformation temperature [1][2][3]. The present work investigates the reactions between Ti and Si in the presence of an ultra-thin Ta interlayer.

Methods and Materials: *In-situ* x-ray diffraction (XRD), resistance measurements and light scattering were used to study the thin film reactions in real time. On both poly-Si and Si(001) substrates Ta thickness was varied from 0 to 1.5 nm while Ti thickness was held constant at ~27 nm.

Results: The time-resolved XRD shows that the volume fraction of C40 and metal-rich silicide phases grows with increasing Ta layer thickness. Increased Ta layer thicknesses also cause delayed growth of the C49 disilicide phase. Among the Ta thicknesses we examined, 0.3 nm is the most effective one in lowering the C49-C54 transformation temperature. Films with Ta layers thicker than 0.5 nm do not completely transform into the C54 phase. The texture of the C54 phase is very sensitive to the Ta thickness. The C54 disilicide film is predominantly (040) textured for the Ti / 0.3 nm Ta sample on both poly-Si and Si(001). The final C54 texture is significantly different for Ta layers thinner or thicker than 0.3 nm. This suggests that the most effective thickness for lowering the C54 formation temperature is related to the development of a strong (010) texture.

Acknowledgments: The authors thank Jean Jordan-Sweet and Steve LaMarra for their help with the *in-situ* experiments. This work was partially supported by NSF ECS-9515181. The National Synchrotron Light Source is supported by the Department of Energy, Division of Materials Science and Division of Chemical Sciences under the contract DOE #DE-AC02-76CH00016.

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